

Hycanthone

Inchi:	InChI=1S/C20H24N2O2S/c1-3-22(4-2)12-11-21-16-10-9-14(13-23)20-18(16)19(24)15-7-
InchiKey:	MFZWMTSUNYWVBU-UHFFFAOYSA-N
Formula:	C20H24N2O2S
SMILES:	CCN(CC)CCNc1ccc(CO)c2sc3ccccc3c(=O)c12
Mol. weight [g/mol]:	356.49
CAS:	3105-97-3

Physical Properties

Property code	Value	Unit	Source
logp	3.661		Crippen Method
mcvol	278.030	ml/mol	McGowan Method
tf	374.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/102-800-9/Hycanthone.pdf>

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